4-Aminopyridine
504-24-5 | DTXSID0023870

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 61.6 °C

Global applicability domain: Inside

Local applicability domain index: 5.25e-01

Confidence level: 6.08e-01

Nearest Neighbors from the Training Set

Image not found
N,N-Dimethyl-p-
phenylenediamine
Measured: 53.0
Predicted: 69.6

Image not found
2-Pyridinecarbonitrile
Measured: 29.0
Predicted: 89.0

Image not found
3-Pyridinecarbonitrile
Measured: 51.0
Predicted: 88.9

Image not found
4-Pyridinecarbonitrile
Measured: 79.0
Predicted: 88.9